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Electrical resistivity of bcc metals

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It is shown that both the anharmonic effects due to isothermal volume expansion and isochoric self-energy of the crystal should be considered in the study of the temperature variation of the electrical resistivity of bcc metals

1 Introduction

In the present paper we have choosen a simple lattice dynamical model to study the temperature variation of the electrical resistivity of bcc metals and it is shown that the electrical resistivity depends on the phonon frequencies. But the temperature dependance of phonon frequencies of a solid is due to two anharmonic effects. Firstly, the isothermal volume expansion of the crystal results in the variation of interatomic force constant, thus contributing to the change in phonon frequences. The frequency shift due to isothermal volume expansion of the solid is obtained by isothermal Grunesen parameter (Grunesen 1926). Secondly, anharmonicity allows phonon—phonon interactions which change the phonon self-energies and also give them a finite life time and since the probability of interaction depends on the phonon occupation number, the phonon frequency and the lifetime will depend on the temperature even when the crystal is kept at constant volume (Cowley & Cowley 1966, Maradudin & Fein 1962, Lowndes 1970 and Tolpadi 1975a, 1975d)

The present investigation on the electrical resistivity of Na, K, Li and Rb shows that both the isothermal volume expansion and isochoric self-energy anharmonic effects should be considered in the study of the temperature variation of phonon frequencies. In the recent studies on the isobaric Grunesen parameter also it has been shown that these anharmonic corrections are necessary for studying the temperature variation of the calorimetric and the X-ray Debye temperatures (Tolpadi 1975c, 1976, 1977)

2 Theoritical Discussion

The starting point of our investigation is the Grunesen-Bloch equation (Meaden 1965), giving electrical resistivity ρ_T at any temperature T. We have

$$\rho_T = \frac{KT}{\rho_2} \, 4 \left(\frac{T}{\theta}\right)^4 \int_0^{\theta/T} \frac{Z^5 \, dZ}{(e^Z - 1)(1 - e^{-Z})} \qquad \ldots \quad (1)$$

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where K is a constant and θ is the relevant Debye temperature of the metal

Eq. (1) may be expressed as

$$\rho_T = KT \frac{G\left(\frac{\theta}{T}\right)}{\theta^2} \qquad .. \quad (2)$$

where $$G\left(\frac{\theta}{T}\right) = 4\left(\frac{T}{\theta}\right)^5 \int_0^{\theta/T} \frac{Z^5 dZ}{(e^Z - 1)(1 - e^{-Z})}$$

For finding the average value of $\frac{G(\theta/T)}{\theta^2}$ we have used Houston's three term formula (Huston 1948 and Betts *et al* 1956) and in the final form the expression for electrical resistivity is

$$\rho_T = \frac{KT}{3}\left[\left(\frac{G_1}{\theta_1^2} + \frac{G_2}{\theta_2^2} + \frac{G_3}{\theta_3^2}\right)\frac{10}{35} + \left(\frac{G_4}{\theta_4^2} + \frac{G_5}{\theta_5^2} + \frac{G_6}{\theta_6^2}\right)\frac{16}{35} + \left(\frac{G_7}{\theta_7^2} + \frac{G_8}{\theta_8^2} + \frac{G_9}{\theta_9^2}\right)\frac{9}{35}\right] \qquad .. \quad (3)$$

where $\theta_1, \theta_2 \ldots \theta_9$ are the Brillouin zone boundary Debye temperatures in the symmetric directions (100), (110) and (111) corresponding to the zone boundary frequencies

The zone boundary frequencies of bcc crystals corresponding to one longitudinal and two transverse modes of vibrations in the directions (100), (110) and (111), assuming that there is no dispersion, is given in table 1. In table 1, $x = \frac{N}{2M}$ where N is the Avogadro number and M is the atomic weight, a is the lattice parameter and C_{11}, C_{12} and C_{44} are the elastic constants of the bcc crystals

Table 1 The zone boundary frequencies of bcc crystals in the specified directions

Direction	Longitudinal wave	Transverse wave	Transverse wave
(100)	$\nu_1 = (C_{11}xa)^{\frac{1}{2}}$	$\nu_2 = \nu_1$	$\nu_3 = (C_{44}xa)^{\frac{1}{2}}$
(110)	$\nu_4 = \left(\frac{(C_{11}+C_{12}+2C_{44})}{4} xa\right)^{\frac{1}{2}}$	$\nu_5 = \nu_2/\sqrt{2}$	$\nu_6 = \left(\frac{(C_{11}-C_{12})}{4} xa\right)^{\frac{1}{2}}$
(111)	$\nu_7 = \left(\frac{(C_{11}+2C_{12}+4C_{44})}{4} xa\right)^{\frac{1}{2}}$	$\nu_8 = \left(\frac{(C_{11}-C_{12}+C_{44})}{4} xa\right)^{\frac{1}{2}}$	$\nu_9 = \nu_8$

3. Results

We have used eq (3) to calculate the electrical resistivity of Na, K, Li and Rb at various temperatures The temperature variation of the zone boundary Debye temperatures was found by using the equations given in table 1, which are based on the elastic constant data (Simon 1971). The method of calculating phonon frequencies by considering the variation of elastic constant data with temperature takes into account the frequency shift due to both the isothermal volume expansion and isochoricself-energy anharmonic effects of the crystal (Tolpadi 1975b, 1975c)

The function G_i ($i = 1, 2, \ldots 9$) which appears in eq. (3) has been obtained from the tables reproduced by Meaden (1965)

The parameter K of eq. (3), which typifies the electron phonon interaction in the metals, was treated a constant for a given metal throughout the range of temperature under consideration and its value was found by accepting the experimental valud of resistivity at 78°K (Meaden 1965)

We have also studied the temperature variation of zone boundary Debye frequencies by considering the anharmonicity due to volume expansion anharmonic effect only. As the elastic constant data were not available at $T \to 0$, we calculated the zone boundary Debye frequency at 78°K. It is assumed that the frequency shift of the 9 Debye frequencies is represented by a single isothermal Grunesen parameter γ_T, defined by

$$\gamma_T = \frac{\alpha_V B_T}{C_V} \quad \ldots, \quad (4)$$

where α, B_T and C_V are the volume expansion coefficient, Bulk modulus of elasticity and specific heat of constant volume respectively.

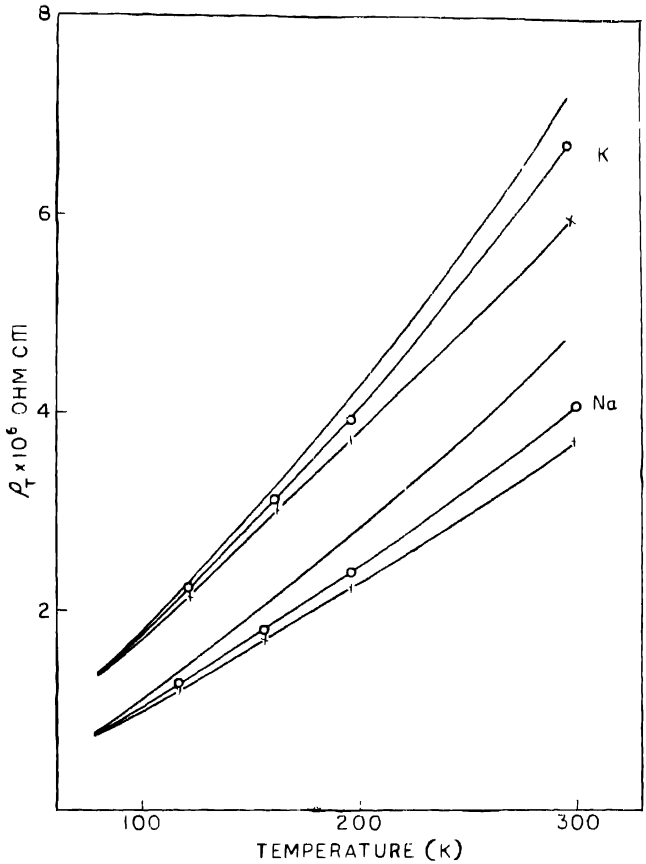
The corresponding frequency shift $\Delta\nu$ due to change in temperature ΔT is given by

$$\Delta\nu = -\gamma_T \nu \Delta V/V = -\gamma_T \nu \alpha \Delta T. \quad \ldots \quad (5)$$

Computing γ_T, using the relevant data (Grey 1972), eq. (5) was now used to obtain the zone boundary frequencies at subsequent temperatures and the resistivity calculated using eq (3). This method of studying the temperature variation of zone boundary frequencies includes the isothermal volume expansion anharmonic effect only and does not take into account the isochoric self-energy anharmonic effect.

Our results (figures 1 and 2) of electrical resistivity of Na, K, Li and Rb show that the resistivity calculated by considering the phonon frequency shift due to both the volume expansion and self-energy anharmonic effects is closer to the experimental value (Meaden 1965) than that calculated by considering

the phonon frequency shift due to volume expansion anharmonic effect only We find that our calculated results in case of Rb are in close agreement with



Fig, 1. Temperature variation of electrical resistivity of sodium and potassium.

the experimental values (l c.), though investigation on Rb could not be made at higher temperatures due to non-availability of elastic constant data. In case of Li our results deviate largely from the experimental results (l c.), which is due to the fact that the Li specimen does not retain the bcc phase throughout the range of temperature (Meaden 1965); but, here too, our main point of investigation is confirmed.

It may be noted that in our earlier study it was found that both the anharmonic effects due to isothermal volume expansion and isochoric self-energy effect must be considered in the study of the temperature variation of the calori-

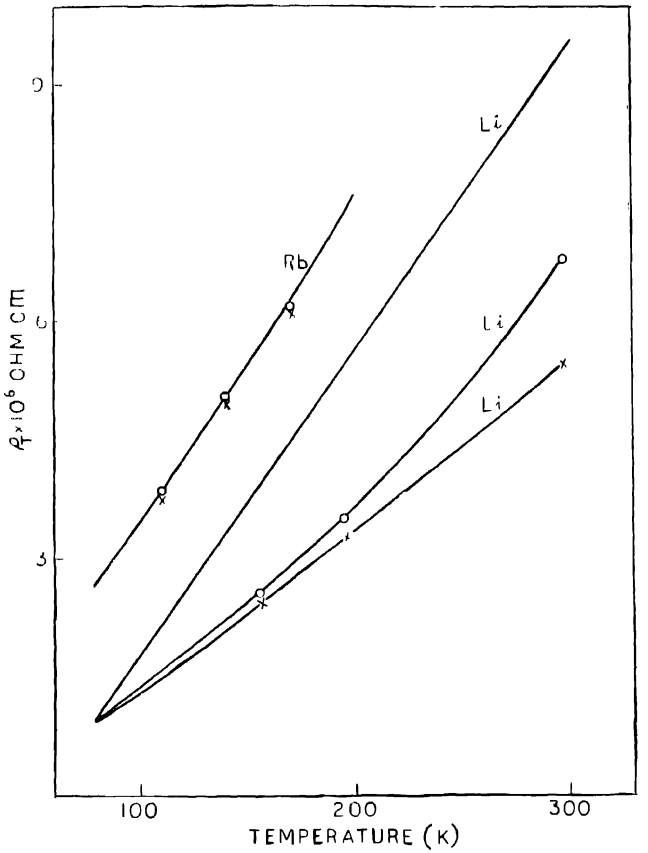


Fig Temperature variation of electrical resistivity of Lithium and Rubidium, [— experimental data (Meaden 1965); -O-O-O- present calculation which includes isothermal and isochoric anharmonic effects, -×-×-×- present calculation considering isothermal anharmonic effect only].

metric and the X-ray Debye temperatures (l c) Our present investigation on electrical resistivity of bcc metals also indicates that both the anharmonic

effects must be taken into account in the study of the temperature variation of phonon frequencies of crystals

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